Осма национална конференција со меѓународно учество - ЕТАИ 2007
Eighth National Conference with International Participation - ETAI 2007
Охрид, Република Македонија - Ohrid, Republic of Macedonia, 19 - 21. IX 2007

THERMAL RELAXATION OF NON-EQUILIBRIUM ELECTRONS IN NANOWIRES

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ABSTRACT

A Wigner function model of early time carrier-phonon dynamics of non-equilibrium carriers confined in nanowire is explored. The presented simulation results reveal effects of collisional broadening, retardation, ultrafast spatial transfer and the intracollisional field effect. These effects characterize thermal relaxation processes which are beyond the Boltzmann assumptions for temporal and spatial locality of scattering.

INTRODUCTION

Quantum wires offer important opportunities as building blocks for the next generation devices ranging from ultrafast optical switchers and highly sensitive photo-FET's, to ultra-dense memories. The electronic characteristics in these systems are basically determined by the carrier transport in the wire. The physical picture corresponds to a locally excited or injected into a semiconductor nanowire carrier package presenting the signal, e.g. an impulse, which evolves under the action of an applied electric field. As a rule, the carrier distribution is highly-nonequlibrium so that besides the usual spatial evolution a thermal relaxation occurs, caused by energy dissipation processes due to phonons. The transport regime is detemined by the nanometer dimensions of the involved structure, the energy of the initial carriers, and the electron-phonon coupling element, which furthermore depends on the temperature and the shape of the wire. A typical non-equilibrium semiconductor carrier can cover a distance of few hundred of nanometers for several hundreds of femtoseconds. Hence carrier transport is characterized by sub-picosecond and nanometer scales and thus requires a quantum mechanical description.

According to the classical (Boltzmann) transport picture point-like carriers move along Newton's trajectories accelerated by the electric field. Their movement is interrupted by scattering events due to the lattice imperfections such as phonons. The scattering events are assumed of having no duration: the carrier momentum is changed by a phonon instantaneously, while the position coordinate remains unchanged. A quantum-mechanical approach shows that these assumptions fail in the discussed transport regime: the electron-phonon interaction can no more be regarded as local in time and space. As obtained, the interaction has a finite duration which is responsible for a number of quantum effects in the carrier evolution. In the next section we introduce a quantum-kinetic equation that is recently derived in [1] to describe the processes of transport and thermal relaxation of carriers in the semiconductor nanowires.

TRANSPORT EQUATION

The equation has been derived from first principle Wigner model of the carrier-phonon system in a quantum wire after a hierarchy of approximations aiming to obtain a closed form for the reduced electron Wigner function f_w:

$$\mathcal{L} f_w(z,k_z,t) = \int dk_z' \int_0^t dt' \left\{ S' f_w' - S f_w \right\} \quad (1)$$

Here $\mathcal{L}$ is the Liouville operator, the Wigner function on the right hand side

$$f' = f_w(\mathcal{Z}(t'), {k_z}'(t'), t')$$

depends on the Newton trajectory

$$z(t') = z - \int_{t'}^{t} \frac{\hbar}{m} k_z(\tau) d\tau, \quad k_z(t') = k_z - \int_{t'}^{t} F(\tau) d\tau$$

initialized at z, k_z, t as follows:

$$\mathcal{Z}(t') = z(t') + \frac{\hbar(k_z - k_z')}{2m}\Delta_c; \quad \Delta_c = t - t'. \quad (2)$$

We note that the electric force $F(t) = qE(t)/\hbar$ can be time dependent but does not depend on the position z. Furthermore $S(k_z, k_z', t, t')$ is obtained from the Boltzmann scattering rate by replacing the energy conserving δ-function

$$\delta(\epsilon(k_z) - \epsilon(k_z') - \hbar\omega)$$

(where $\epsilon(k_z)$ and $\epsilon(k'_z)$ are the carrier energies before and after the scattering by a phonon with energy $\hbar\omega$) by

$$\mathcal{D} = \frac{1}{2}exp\left(-\int_{t'}^{t}\Gamma\left(\frac{k_z(\tau)+k'_z(\tau)}{2}\right)\right)\times \quad (3)$$
$$cos\left(\int_{t'}^{t}\left(\frac{\epsilon(k_z(\tau))-\epsilon(k'_z(\tau))-\hbar\omega}{\hbar}\right)d\tau\right)$$

Γ is the total Boltzmann out-scattering rate, S and f_w are obtained from S' and f' by exchanging of the primed and unprimed momentum variables. The main factors which outline the transport model (1) from the classical Boltzmann equation are:

- The existense of the time integral on the right hand side of (1);
- The function (3) which replaces the classical energy conserving delta function in the scattering operator S;
- The time interval Δ_c identified as the collision duration time. The later is zero in the classical case so that the quantum trajectory $\mathcal{Z}(t')$ reduces to the classical Newton's trajectory $z(t')$.

These factors introduce a number of quantum phenomena in the carrier-phonon kinetics, demonstrated by the evolution of the the Wigner function and its first moments - the carrier density, energy and wave vector distributions. Here we summarize the introduced effects:

i The non-Markovian character of the equation introduced by the time integral leads to retardation of the quantum evolution.

ii The lack of energy conservation causes collisional broadening and appearance of carriers in the classically forbidden energy regions. The spatial manifestation of the broadening is ultrafast spatial transfer (UST): existence of quantum carriers which reach larger distances than the fastest classical carriers.

iii Collisions with phonons have finite duration Δ_c which affects the carrier trajectories (2). It can be shown that if this time is neglected, the evolution becomes unphysical.

iv The action of the electric field during the collision process-the so called Intra-Collisional Field Effect (ICFE). The electric field significantly influences the carrier-phonon kinetics, which, moreover, depends on the direction of the electric force.

These phenomena must be taken into account in the next generation simulators of transport processes occurring on femtosecond and nanometer scales. In the next section we analyse some of these phenomena with an emphasis on the momentum subspace where the energy transfer between the hot carriers and the phonons gives rise to thermal cooling of the carrier system.

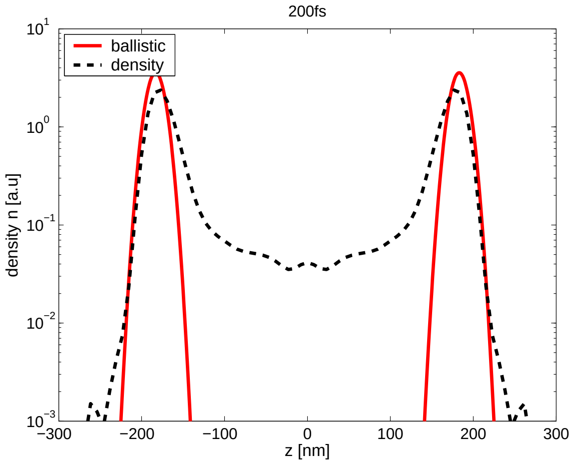

Fig. 1. Carrier density $n(z)$ after 200fs evolution.

SIMULATION RESUTLS AND ANALYSIS: THERMAL RELAXATION

The transport equation (1) is solved by a backward Monte Carlo method for the following physical conditions. A GaAs wire with 10 nm square cross section is considered. The carriers are assumed in the Gamma valley, a single optical phonon with a constant energy is considered in the semiconductor model. The initial carrier distributiion corresponds to a Gaussian distribution both in energy and space that is generated by a laser pulse with $150meV$ excess energy. As the shape of the wire affects the carrier-phonon coupling via the carrier state and band in the plane normal to the wire, we filter out the effects of the interband transitions by a choice of a very low temperature, which fixes the carriers in the ground state in the plane. This is in accordance with (3), where the interband energies are excluded.

The evolution of the carriers occurs both in the real z and in the momentum $p_z = \hbar k_z$ parts of the phase space. We briefly discuss the spatial evolution of the carriers in the case of no electric field applied along the wire. The carrier distribution, initially centered at $z = 0$, splits into two peaks which move in directions of $\pm z$. The carrier density

$$n(z) = \int f_w(z, k_z)dk_z$$

after 200 fs evolution is shown in Fig. 1 and is compared with the ballistic curve. The latter is obtained by turning off the phonon interaction. In the central

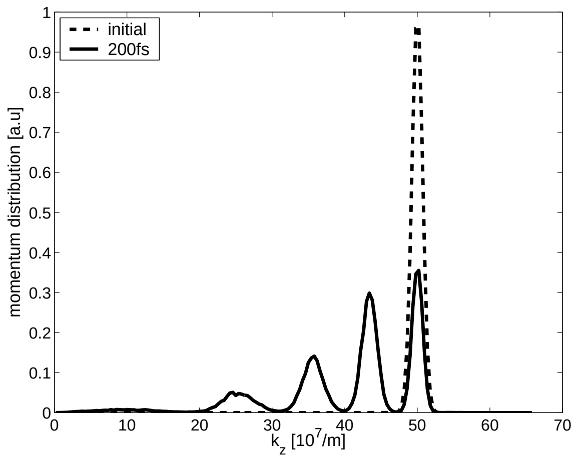

Fig. 2. Momentum distribution obtained by the long time limit of equation (1).

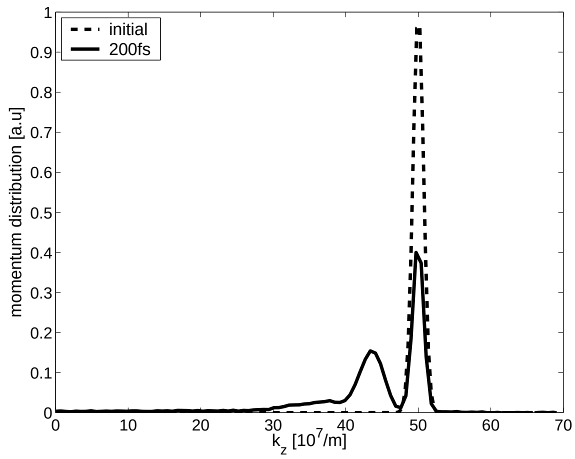

Fig. 3. Momentum distribution at 200fs obtained from equation (1).

region carriers are slowed down by the scattering events. More interesting is the effect of UST: a finite density of quantum carriers reach distances further away from the origin. As the front ends of the ballistic peaks are comprised by the fastest classical carriers, this is an entirely quantum phenomena. The UST effect is associated with the lack of energy conservation in the interaction process: some carriers gain energy from the collisions and thus increase the velocity due to the scattering.

In the momentum subspace occur processes of energy transfer: both the applied electric field and the phonon scattering change the wave vector k_z of the carriers. We first discuss the zero field case. The choice of a very low temperature provides a clear classical picture which is used as a reference for the quantum effects. At $T = 0$K classical carriers can only emit phonons and since the chosen constant PO energy give rise to replicas of the initial condition. The consecutive replicas correspond to emission of one phonon (first replica), a second phonon (second replica), etc. This is illustrated in Fig. 2 presenting the momentum distribution at 200fs *as obtained for the long time limit of the equation.* This limit is briefly discussed in the Appendix; here we note that the solution of the Boltzmann equation is basically the same. The physical meaning of the curve is as follows: the peaks correspond to the number of carriers, equally spaced in energy, with the highest energy - this of the initial condition - to the most right at wave vector value of 50 [10^7/m]. The region slightly above this value is voted from carriers and remains classically forbidden as only phonon emission is possible. Moreover, since the mean time between the collisions is about 50fs, at least tree replicas are formed after 200fs of the Markovian evolution. This gives a measure of the thermal energy transferred to the lattice. The more is the number of the replicas, the smaller is the averaged kinetic energy of the carrier system.

In contrast to its long time limit, the general quantum-kinetic equation (1) is non-Markovian: To obtain the solution at time t one needs the solutions at all times $t' < t$ due to the time integral on the right. The non-Markovian evolution gives rise to a significant retardation of the processes of electron cooling. The momentum distribution

$$f(k_z) = \int f_w(z, k_z) dz$$

shown on Fig. 3 reveals only one well formed replica for the same evolution time of 200fs. Thus, according to the quantum model, the averaged carrier is well above the classical counterpart. Accordingly, the signal which evolves along the wire conserves a larger part of the initial coherence in energy. Another peculiarity of the quantum model is the broadening of the replicas which is time dependent. This is shown in Fig. 4 with the momentum distribution at 60 and 160 femtoseconds. The first replica is very broadened at 60fs. A finite carrier density exists in the region to the right of the initial peak, above 52×10^7[m^{-1}], in the region which is classically forbidden. The appearance of carriers in this region is associated with the lack of energy conservation at the initial stages of the electron-phonon interaction. With the increase of the time, processes obeying energy conservation begin to dominate. The initial peak becomes well pronounced at $160fs$ but remains much wider as compared to the initial peak.

Finally we discuss the role of the electric force

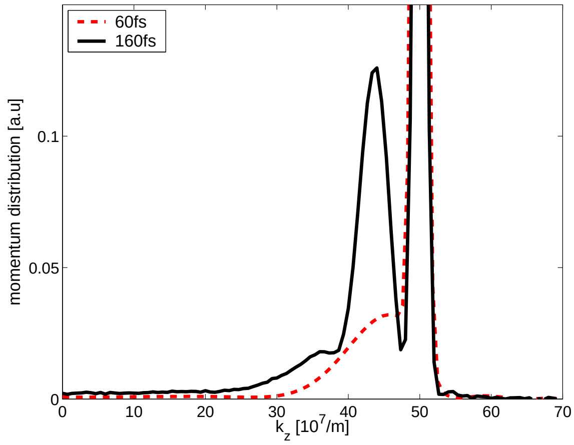

Fig. 4. Momentum distribution at two different evolution times.

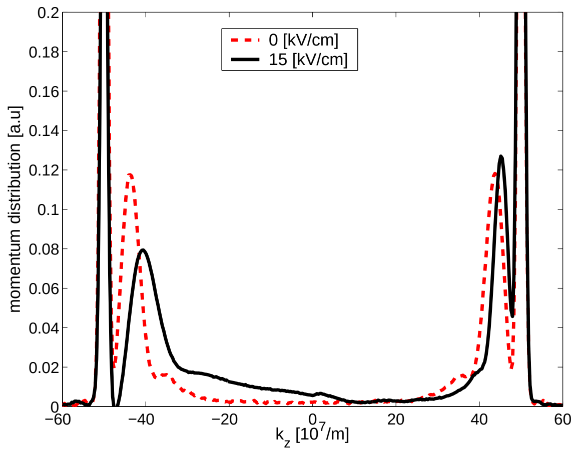

Fig. 5. ICFE in nanowire: momentum distribution after 150fs evolution.

during the electron-phonon interaction, giving rise to ICFE. The electric force points to the right. The zero field curve, which is symmetric with respect to the origin, is used as a reference. A comparison is possible as the 15[kV/cm] curve is presented according to a coordinate system accelerated by the force. For carriers traveling against the force, a virtual increase of the phonon energy occurs as well as an increase of the collisional broadening. Along the force, the phonon energy effectively decreases in addition to the broadening effects. In this direction the electric force reduces the dissipation processes and thus helps to conserve the coherence of the signal.

CONCLUSIONS

Nanowires are used a building blocks in some modern nanoelectronic devices. The electronic characteristics of these systems depend on the carrier transport in the nanowire, which is characterized by the ultimate nanometer and femtosecond scales. Some of the basic notions of the classical transport picture fail at such scales so that a quantum description is necessary. A quantum-kinetic equation, previously derived to provide more realistic description of the carrier behaviour in nanowires, is now used to explore the thermal relaxation of the carriers caused by the interaction with the lattice vibrations. The equation is solved for an initial condition - a packet of hot carriers which can be associated with an impulse initiated in the wire. The obtained simulation results demonstrate that at the early stages of the electron-phonon kinetics there are effects of retardation and collision broadening. The transfer of the carrier energy to the lattice is slowed down which preserves for longer time the initial coherence of the signal. The applied electric field affects this process in a directionally dependent way: The ICFE effectively reduces the phonon energy in the direction of the field, while in the opposite direction the phonon energy is increased. These typically quantum phenomena must be taken into account in the next generation device simulators.

I. APPENDIX

The long time limit of (1) can be analytically calculated [2] if there is no spatial dependence. That is, in the homogeneous case if the upper bound t of the integral on the right is replaced by infinity and the equation is expressed in its integral form, the time integration can be carried on explicitly, giving rise to a Lorentzian. Then the scatering kernel S contains a Lorentzian in the place of the classical delta function. Nevertheless, the evolution becomes Markovian: the solution at given time t can be obtained by using the solution at any given time $0 < t' < t$ as an initial condition (at time t'!). There is no memory about the events which occur at times smaller than t'. The homogeneous Boltzmann equation is furthermore recovered if in addition Γ in (3) is let to zero. The distribution on Fig. 2 is obtained for the case of $\Gamma \neq 0$. However as the corresponding value for $GaAs$ is small, the behavior of the curve is the same as in the Boltzmann limit.

ACKNOWLEDGEMENTS

One of the authors (MN) would like to acknowledge the support from Österreichische Forschungsgemeinschaft (ÖFG), Project MOEL239.

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